National Center for Computational Sciences Snapshot The Week of February 5, 2007

Move to XT4 is at Hand

Jaguar users will soon be able to use the new 68-cabinet XT4 system on the second floor of the Computational Sciences Building in anticipation of system upgrades to 100 teraflops and eventually 250 teraflops.

The new system, which features more than 6,000 dual-core AMD Opteron processors, is currently undergoing acceptance testing. When the testing is completed in early February, users will be allowed to migrate to the new system, a process that is expected to take about a week.

Once that migration has been completed, the existing XT3 cabinets will be moved from the first floor to the second floor; the two systems will then be connected and merged into one, creating a single system capable of more than 100 teraflops.

The upgrade to 250 teraflops is expected around the end of the year. At that time, the dual-core processors will be replaced with quad-core processors, the memory will be doubled, and the operating system will migrate to a stripped-down version of Linux on the compute nodes.

The NCCS is working with users to minimize the inconvenience caused by these upgrades, providing regular status updates and guidance for the transition. The system is expected to be unavailable for about 3 weeks when the XT3 and XT4 systems are merged. Significant downtime is also expected with the upgrade to 250 teraflops.

While the downtimes associated with these upgrades are unfortunate, they are necessary as the NCCS continues to provide the most powerful supercomputers in the nation for open scientific research. The NCCS is committed to ensuring that disruptions brought about by these upgrades are as small as possible.

Kothe Speaks to Cray Conference in Tokyo

National Center for Computational Sciences (NCCS) Director of Science Doug Kothe had an opportunity recently to share the center's computing accomplishments with Japan's high-performance computing (HPC) community.

Kothe gave an invited talk entitled "Science Enabled by Leadership Computing—Science Highlights and Outlook at the ORNL Leadership Computing Facility" at the fourth Cray HPC conference 2007, held January 25 and 26 in Tokyo.

The conference gave him an opportunity to share the cutting-edge computing accomplishments of the NCCS both with manufacturers and developers and with potential users in Japan.

"Science is an international thing," he noted, "so we want to embrace the talent wherever it is. Places like Toyota and other Japanese companies are either engaged in HPC or interested in getting into the game."

The conference also gave Kothe an opportunity to highlight the leadership role that the Oak Ridge center has taken on in supercomputing.

"I think that DOE and the LCF [Leadership Computing Facility] here, jointly with Cray, are among the world leaders when it comes to high-performance computing," he said.

NCCS Staffer Discusses Computing with Birmingham College Students

The future looks bright for tomorrow's computational scientists and other information technology professionals.

That was one of the messages Tom Barron of the NCCS Technology Integration Group was able to deliver recently to a group of college students and faculty in Birmingham, Alabama. Barron was in Birmingham as the keynote speaker for a symposium hosted by the Birmingham Area Consortium for Higher Education (BACHE), a cooperative effort among the city's 4-year colleges and universities. The BACHE Scholars in Computer Science and Mathematics Symposium was held at Birmingham-Southern College.

"It's an excellent field to be in," said Barron, who used information from sources such as the Department of Commerce, the National Science Foundation, the College Board, and *Fortune* magazine to demonstrate that the upcoming job market for computing professionals promises to be stronger than both the overall job market and that for science and technology as a whole.

Before Barron's keynote, the group heard presentations from several students who talked about research they had performed. One explained a project in artificial intelligence that analyzed the frequency of one-, two-, and three-word groups in text. Another discussed an effort to produce an algorithm for playing the board game "Othello," in which players take turns placing stones on a board and attempt to "outflank" one another. A third discussed the creation of an algorithm that creates a curve from a series of points on a graph. And a team of two students discussed their attempt to build a robot that can analyze an image well enough to recognize itself. All told, there were seven student presentations.

Barron reviewed computational science in general, outlined research being conducted at Oak Ridge National Laboratory (ORNL), and explained the preparation expected of a student interested in joining the field. He also outlined opportunities being offered at ORNL, focusing especially on internships.

Barron gave the talk as a participant in ORNL's Speakers Bureau. He recently joined the bureau, which provides Lab professionals to talk to civic and community groups in the region, because he has a long-standing fondness for public speaking.

"I've been in Toastmasters a couple of different times," he explained, "once in Nashville and for a while here in Oak Ridge. I enjoy that kind of opportunity, that kind of involvement, and when the Speakers Bureau idea turned up, I jumped on it."

His enthusiasm and knowledge paid off, according to symposium organizer Marietta Cameron of Birmingham-Southern's computer science faculty.

"The students got to hear about the importance of computational sciences from someone besides the usual suspects," she said. "Some of them are very excited about the opportunities at Oak Ridge.

"The students found him very engaging, and they want him to come back," she said.